Monte Carlo Modeling of the X–Valley Leakage in Quantum Cascade Lasers

X. Gao, D. Botez, and I. Knezevic
Department of Electrical and Computer Engineering, University of Wisconsin – Madison,
1415 Engineering Dr, Madison, WI 53706-1691, USA
e-mail: xujiaogao@wisc.edu, knezevic@engr.wisc.edu

Room-temperature, pulsed mode operation of a 9μm GaAs/AlGaAs quantum cascade laser (QCL) has been accomplished by increasing the Al content from 33% to 45% within the conventional three-well active region design [1]. This important milestone in the mid/far-infrared QCL technology was achieved due to the ~95 meV larger band offset in the 45% Al structure, which suppressed thermal leakage into the continuum states and significantly improved the temperature dependence of the threshold current. However, Al content of 45% or above is also expected to result in appreciable carrier leakage into the X-valley subbands [2, 3], but has not yet been accounted for in theoretical predictions [2-4].

In this paper, we present the first numerical simulation of X valley leakage in GaAs/AlGaAs QCLs [5]. The Monte Carlo QCL simulator we developed is based on solving the microscopic Boltzmann-like transport equation of Ref. [4], but also incorporates the X valley transport. The wavefunctions and energy levels in both Γ and X valleys are obtained by self-consistently solving the coupled 1D Schrödinger and Poisson equations. The Schrödinger equation for the Γ valley is solved using the 3-band **k.p** method within the envelop function and effective mass approximations. For the X valley subbands, the usual effective mass equation for the conduction band is sufficient, since the X valleys are well above the valence bands. The self-consistent Schrödinger-Poisson solver results in the wavefunctions and energy levels of the conduction subbands in both valleys, which are then used as input for the 3D Monte Carlo transport kernel.

The Monte Carlo transport simulation is based on the technique introduced in [4], with both the Γ and X valley transport included. In addition to the intersubband (including inter-stage and intra-stage) and intrasubband electron-LO and electron-electron scattering mechanisms within the Γ valley [2,3], we also include the Γ-X and X-X intervalley scattering, and the inter- and intra-subband electron-LO scattering mechanisms in the X valleys.

In Fig. 1, we present the calculated electric field vs. current density for the extensively simulated [2, 3], 36-stage GaAs/$Al_{0.45}Ga_{0.55}As$ QCL structure introduced in Ref. [1]. The simulations were done at low (77 K) and high temperatures (300 K), both with and without the X valley transport included. At both temperatures, the results from our Monte Carlo simulator without the X valley transport agree with the data from Ref. [2]. At low temperature, the increase in current density due to X-valley leakage is small. At room temperature, however, Γ-X intervalley scattering becomes strong, and the parallel current path through the X valley leads to a significant increase in the current density for a given electric field.

In summary, we have presented the first Monte Carlo simulation incorporating the effects of the X-valley leakage on the operation of GaAs-based QCLs. This realistic simulator can also be adapted to account for the indirect valley leakage in InP-based structures, thereby becoming a versatile aid in the design of mid and far-infrared QCLs.

This work is supported by the Wisconsin Alumni Research Foundation (WARF).

[1] H. Page, C. Becker, A. Robertson, G. Glastre, V. Ortiz, and C. Cirtori, Appl. Phys. Lett. **78**, 3529 (2001).
[2] A. Mircetic, D. Indjin, Z. Ikonic, P. Harrison, V. Milanovic, and R. W. Kelsall, J. Appl. Phys. **97**, 084506 (2005).
[3] D. Indjin, P. Harrison, R. W. Kelsall, and Z. Ikonic, Appl. Phys. Lett. **81**, 400 (2002).
[4] R. C. Iotti, and F. Rossi, Phys. Rev. Lett. **87**, 146603 (2001).
[5] X. Gao, D. Botez, and I. Knezevic, *in preparation.*

ISBN 3-901578-16-1

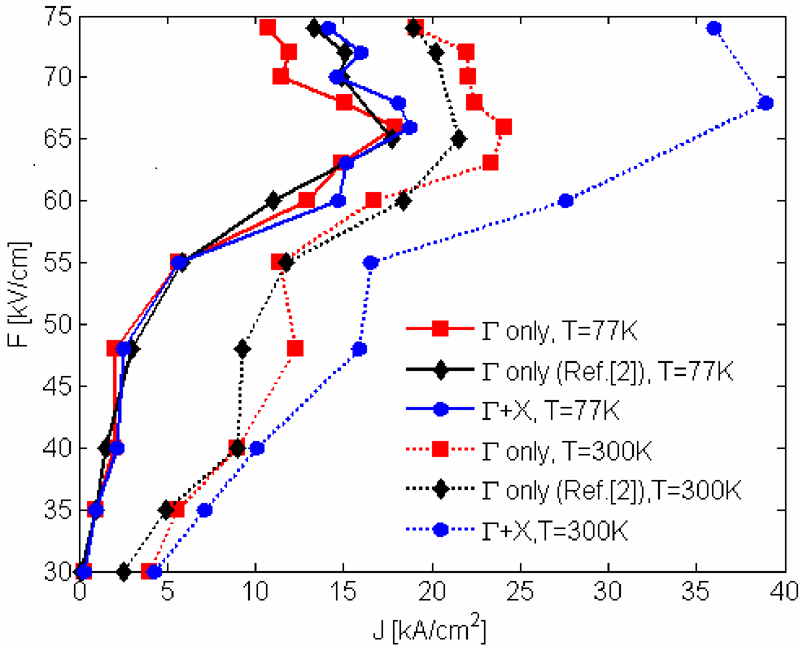

Fig. 1. Electric field vs. current density characteristics for the GaAs/$Al_{0.45}Ga_{0.55}As$ structure introduced in Ref. [1], at T = 77 K and T = 300 K, with and without X valley transport included. The simulation results without the X-valley leakage agree with those previously obtained for the same structure by Mircetic *et al.* [2], who used a self-consistent solution of the rate equations. At low temperature, it is clear that X-valley leakage does not play a major effect in the QCL performance. Although the 45% Al content of this structure suppresses thermal leakage of carriers into the continuum states, we see that the X-valley leakage becomes appreciable at room temperature.